Supplementary Information

Evaluation of a Rapid Biosensor Tool for Measuring PAH Availability in Petroleum-Impacted Sediment

1. Sediment Preparation and Bulk Chemistry

Following receipt of samples from the field, the sediments were inspected and homogenized with a handheld mixer and separated into 250-mL amber glass wide-mouth jars for storage at 4°C until analysis.

Two jars from each of the four sediments were used for analysis of bulk chemistry parameters via United States Environmental Protection Agency (USEPA) SW-846 methods at a commercial chemical analytical laboratory (TestAmerica). Parent and alkylated PAHs (35 analytes, Table S1) were analyzed via Gas Chromatography/Mass Spectrometry Isotope Dilution methods consistent with USEPA Method 8270 (USEPA, 2018). This analytical program included all 34 PAHs typically measured in assessments for sites at which USEPA is the regulatory authority, although our analyses were able to report benzo[b]fluoranthene and benzo[k]fluoranthene as individual analytes instead of the combined "benzo[b+k]fluoranthene" analyte (sum of benzo[b]fluoranthene and benzo[k]fluoranthene) sometimes reported in other investigations (Hawthorne et al., 2006). Total Petroleum Hydrocarbons (TPH) analytes TPH Diesel Range, TPH Oil Range, and TPH Gasoline Range were analyzed via USEPA Method 8015C (USEPA, 2007). Total Organic Carbon (TOC) and Black Carbon (BC) contents were measured via Lloyd Kahn method (USEPA, 1988). Notes from the inspection of the sediment and results of the bulk chemistry analysis (concentrations on a dry weight sediment basis) are shown in Table S2.

In addition, each sediment was also evaluated for the concentration of Total PAHs (ΣPAH), TPH Diesel Range, TPH Oil Range, and TPH Gasoline Range via the UVF-Trilogy a commercially available benchtop screening module available from Site-Lab (http://site-lab.com/index.htm). Procedures available from the manufacturer were used. Briefly, 5 grams (wet weight, ww) of sediment sample were weighed into an extraction vial, to which 10 mL of methanol (for PAHs, TPH Diesel Range, and TPH Gasoline Range) or 10 mL hexane (for TPH Oil Range) was added. Following shaking of the vial for several minutes, the solvent was diluted with additional solvent to comprise several diluted solutions that were placed in a cuvette and analyzed via insertion into the analyte-specific module housed with the UVF-Trilogy analyzer, which reported the concentration in the solid sample on a mg analyte/kg sediment basis. Analyses of ΣPAH, TPH Diesel Range, and TPH Oil Range were conducted twice – once by our research team (Analysis 1) and once by the device manufacturer (Site-Lab, Analysis 2). TPH Gasoline Range was only tested by Site-Lab due to limited availability of the TPH Gasoline Range module. Overall, the correlations between UVF-Trilogy results and the USEPA SW-846 methods for the four test sediments were marginal for the TPH and PAH analytes (Figure S1). Note that some minor discrepancy would be expected due to the fact that the concentrations determined via UVF-Trilogy values may be expected to be somewhat lower since they are on a wet weight basis.

Table S1. Polycyclic Aromatic Hydrocarbons (PAHs) measured in this study.

Name	CAS Number	Rings	Parent or Alkylated	Group	Abbrev-iation
Naphthalene	[91-20-3]	2	Parent	Naphthalenes	N0
1-Methylnaphthalene	[90-12-0]	2	Alkylated		N1-1
2-Methylnaphthalene	[91-57-6]	2	Alkylated		N1-2
C1-Naphthalenes*		2	Alkylated		N1
C2-Naphthalenes		2	Alkylated		N2
C3-Naphthalenes		2	Alkylated		N3
C4-Naphthalenes		2	Alkylated		N4
Acenaphthylene	[208-96-8]	3	Parent		Acl
Acenaphthene	[83-32-9]	3	Parent		Ace
Fluorene	[86-73-7]	3	Parent	Fluorenes	F0
C1-Fluorenes		3	Alkylated		F1
C2-Fluorenes		3	Alkylated		F2
C3-Fluorenes		3	Alkylated		F3
Anthracene	[120-12-7]	3	Parent	Phenanthrenes & Anthracenes	AN
Phenanthrene	[85-01-8]	3	Parent		P0
C1-Phenanthrenes/Anthracenes		3	Alkylated		P1
C2-Phenanthrenes/Anthracenes		3	Alkylated		P2
C3-Phenanthrenes/Anthracenes		3	Alkylated		P3
C4-Phenanthrenes/Anthracenes		3	Alkylated		P4
Fluoranthene	[206-44-0]	4	Parent	Fluoranthenes and Pyrenes	FL
Pyrene	[129-00-0]	4	Parent		PY
C1-Fluoranthenes/pyrene		4	Alkylated		FP1
Benzo[a]anthracene	[56-55-3]	4	Parent	Chrysenes & Benz(a)anthracenes	BaA
Chrysene	[218-01-9]	4	Parent		C0
C1-Chrysenes/Benz[a]anthracenes		4	Alkylated		C1
C2-Chrysenes/Benz[a]anthracenes		4	Alkylated		C2
C3-Chrysenes/Benz[a]anthracenes		4	Alkylated		C3
C4-Chrysenes/Benz[a]anthracenes		4	Alkylated		C4
Benzo[b]fluoranthene	[205-99-2]	5	Parent		BbF
Benzo[k]fluoranthene	[207-08-9]	5	Parent		BkF
Benzo[e]pyrene		5	Parent		BeP
Benzo[a]pyrene	[50-32-8]	5	Parent		BaP
Perylene		5	Parent		Per
Dibenz[a,h]anthracene	[215-58-7]	5	Parent		DA
Indeno[1,2,3-cd]pyrene	[193-39-5]	6	Parent		ID
Benzo[g,h,i]perylene	[191-24-2]	6	Parent		BgP

Notes

*: Sum of 1-methylnapthylene and 2-methylnapthylene measured values.

Table S2. Description and bulk chemistry results for the four test sediments. Where not detected, the MDL ("< value") are reported.

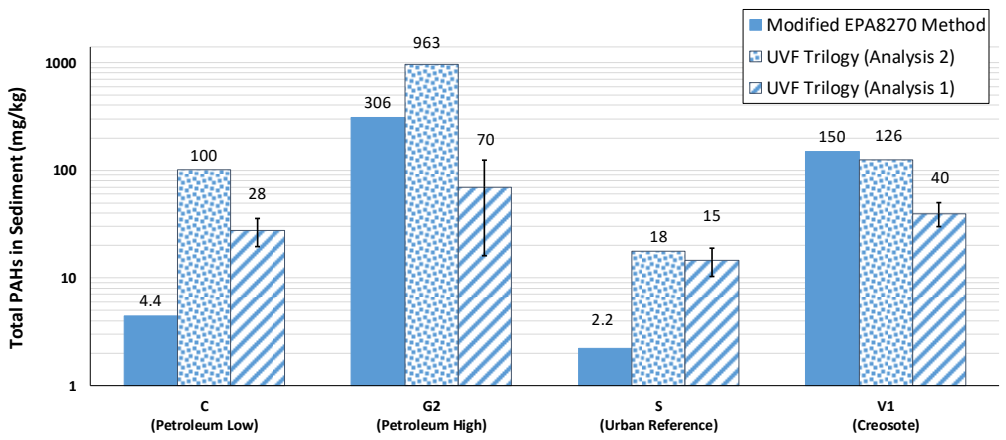
Analyte	Units	C (Petroleum Low)	G2 (Petroleum High)	S (Urban Reference)	V1 (Creosote)
Site description and PAH source	NA	Freshwater, petroleum PAHs	Estuarine, petroleum PAHs	Freshwater, Urban area with no distinct PAH sources	Estuarine, creosote PAHs
Sediment texture (Tactile evaluation)	NA	Sandy silt	Clayey silt	Silty sand	Sandy with a trace of silt
Non-Aqueous Phase Liquid (NAPL)?	NA	No	Visible	No	Visible
Visible sheen or petrol odor?	NA	Odor, but no sheen	Sheen and odor	No	No
Total Organic Carbon (TOC) Content	%	0.58%	7.4%	4.1%	0.52%
Black Carbon (BC) Content	%	0.23%	0.60%	0.55%	0.13%
Naphthalene	mg/kg	0.013	0.52	0.11	4.5
1-Methylnaphthalene	mg/kg	0.016	0.33	0.025	1.1
2-Methylnaphthalene	mg/kg	0.043	0.72	0.04	3.2
C2-Naphthalenes	mg/kg	0.083	37	0.074	2.1
C3-Naphthalenes	mg/kg	0.2	62	0.082	1.2
C4-Naphthalenes	mg/kg	0.31	50	0.086	0.45
Acenaphthylene	mg/kg	0.0047	0.71	0.017	0.38
Acenaphthene	mg/kg	0.0025	0.45	0.019	2.1
Fluorene	mg/kg	0.0069	1.5	0.036	7.8
C1-Fluorenes	mg/kg	0.03	7.6	0.027	0.93
C2-Fluorenes	mg/kg	0.15	29	0.048	0.57
C3-Fluorenes	mg/kg	0.23	26	0.091	0.42
Anthracene	mg/kg	0.09	0.66	0.048	61
Phenanthrene	mg/kg	0.041	4.6	0.23	14
C1-Phenanthrenes/Anthracenes	mg/kg	0.14	9.5	0.19	2.1
C2-Phenanthrenes/Anthracenes	mg/kg	0.45	25	0.1	1.6
C3-Phenanthrenes/Anthracenes	mg/kg	0.46	21	0.26	0.84
C4-Phenanthrenes/Anthracenes	mg/kg	0.22	12	0.18	0.32
Fluoranthene	mg/kg	0.016	1	0.17	9.1
Pyrene	mg/kg	0.1	0.85	0.12	8.5
C1-Fluoranthenes/pyrene	mg/kg	0.22	2.8	0.055	5
Benzo[a]anthracene	mg/kg	0.045	0.36	0.028	3.2
Chrysene	mg/kg	0.044	1.3	0.034	3.4
C1-Chrysenes/Benz[a]anthracenes	mg/kg	0.21	3	0.025	2.8
C2-Chrysenes/Benz[a]anthracenes	mg/kg	0.22	3.4	0.022	1.1
C3-Chrysenes/Benz[a]anthracenes	mg/kg	0.26	2.7	0.014	0.43
C4-Chrysenes/Benz[a]anthracenes	mg/kg	0.19	1.8	0.0086	0.17
Benzo[b]fluoranthene	mg/kg	0.031	0.21	0.025	3.8
Benzo[k]fluoranthene	mg/kg	0.012	< 52	0.013	2
Benzo[e]pyrene	mg/kg	0.12	0.19	0.017	2
Benzo[a]pyrene	mg/kg	0.051	0.15	0.019	2.8
Perylene	mg/kg	0.0075	0.59	0.15	0.76
Dibenz[a,h]anthracene	mg/kg	0.035	0.041	0.0024	0.45
Indeno[1,2,3-cd]pyrene	mg/kg	0.059	0.061	0.0086	1.2
Benzo[g,h,i]perylene	mg/kg	0.45	0.14	0.029	1.3
Total PAHs (ΣPAH)	**mg/kg**	**4.6**	**307**	**2.4**	**153**
Total Parent PAHs	**mg/kg**	**1.1**	**13**	**1.1**	**128**
Total USEPA Priority Pollutant (Parent) PAHs	**mg/kg**	**1.0**	**13**	**0.91**	**126**
TPH (Diesel Range)	mg/kg	220	16000	280	180
TPH (Oil range)	mg/kg	330	15000	330	140
TPH (Gasoline Range)	mg/kg	< 80	180	< 25	< 63
Total TPHs	**mg/kg**	**550**	**31180**	**610**	**320**

Notes

NA: Not Available

Summed "Total" values were calculated by summing the detected analytes.

(a)



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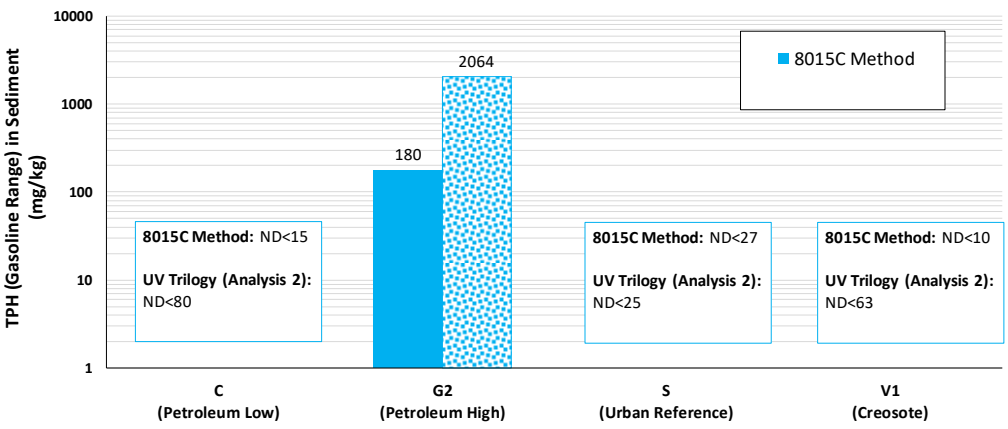

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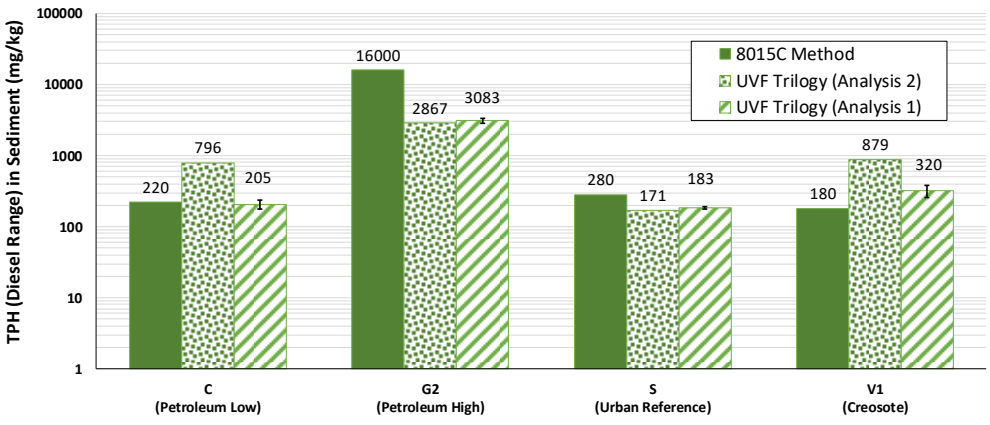

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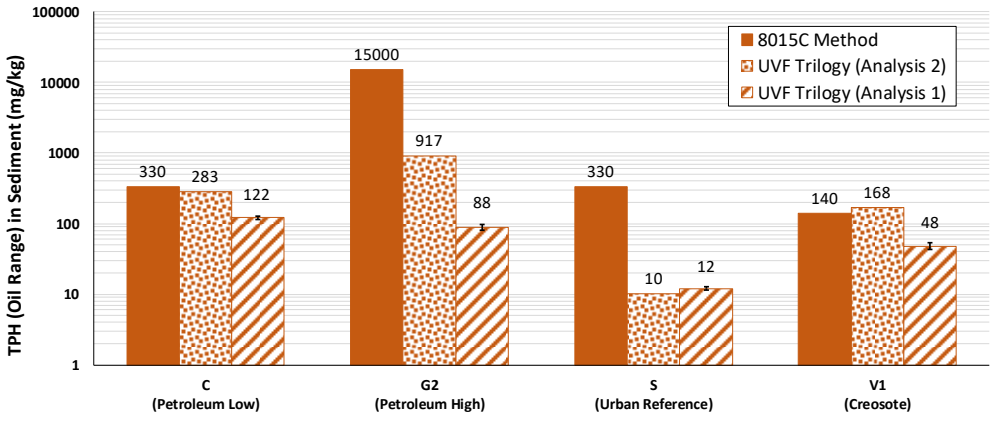


(e)

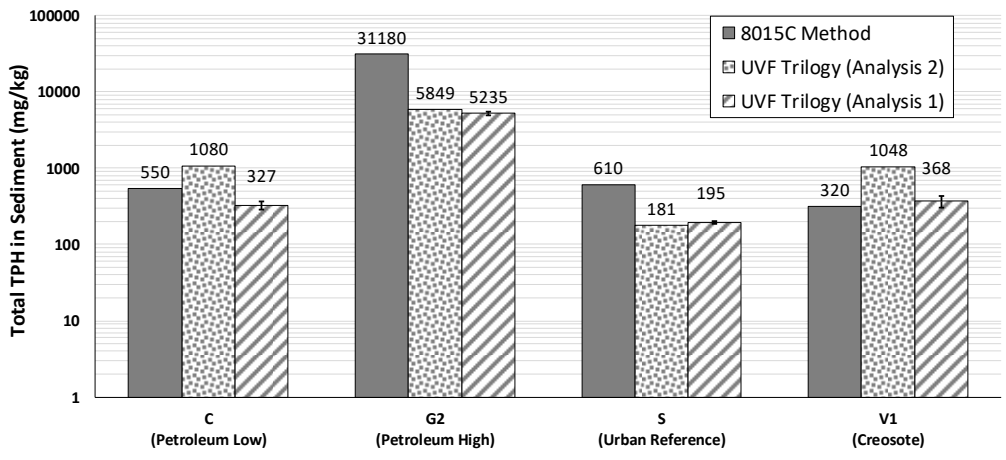


Figure S1. Concentration of total PAHs (a), TPH Gasoline Range (b), TPH Diesel Range (c), TPH Oil Range (d), and total TPH (e) in the four test sediments, as measured by conventional USEPA-SW846 Methods (USEPA 8270 and USEPA 8015C) and the benchtop UVF Trilogy module. Results are measured values (USEPA-SW846 Methods and UVF Trilogy Analysis 2) or mean (SD) for UVF Trilogy Analysis 1.

2. Additional C_{free} Measurement Detail and Raw Data

Additional Biosensor Measurement Detail and Raw Data
Porewater volumes required for the biosensor method used for these analyses (Li et al, 2016) are low (1-5 mL) and can usually be obtained via allowing sediment samples to settle, centrifuging (Hartzell et al. 2018), or a mechanical sediment compression apparatus. As noted in the main text, the initial porewater aliquot of sample V1 did not contain sufficient recoverable porewater, so an additional aliquot was prepared from the sediment slurry that had been used for the passive sample analysis (250 mL of wet sediment and 250 mL ultrapure water that were equilibrated via end-over-end mixing for 28 d, as described in the subsection below).

Multiple biosensor C_{free} ΣPAH measurements were made on each sediment (Table S3), and the mean value of the multiple measurements were used for subsequent data analysis.

Table S3. Freely-dissolved PAH concentration (C_{free}) of the PAHs (ΣPAH) as determined by biosensor in the four test sediments.

Sediment	Porewater Sample	Fine-particulates present? (sample was 0.45-µm filtered)	Total ΣPAH C_{free} (µg/L)		
			Value	Average	SD
C	Si-4006-C rep A	Yes	4.14	4.3	0.22
	Si-4006-C rep B	Yes	4.45		
G2	Si-4006-G2 rep A		55.31	55	0.21
	Si-4006-G2 rep B		55.60		
S	Si-4006-S rep A	Yes	2.93	3.1	0.18
	Si-4006-S rep B	Yes	3.18		
V1	Si-4006-V1 rep A		18.3	20	1.5
	Si-4006-V1 rep B		18.36		
	Si-4006-V1 rep C		21.47		
	Si-4006-V1 rep D		20.09		

Notes
SD: Standard Deviation

Additional Passive Sampler and Raw Data
The passive samplers used in this project were SP3™ passive samplers provided by SiREM (https://www.siremlab.com/, Guelph, Ontario, Canada), and methods described below are consistent with passive sampling practices recommended by SERDP/ESTCP and USEPA (2016) and techniques developed by the lead author over the last 20 years (Conder et al., 2003). The SP3™ sampler design for this project consisted of a 3 centimeter (cm) × 3 cm sheets of 13 micrometer (µm) thick low-density polyethylene (PE) housed in a stainless-steel mesh envelope. For all SP3™ the solvent cleaned PE was spiked with Performance Reference Compounds (PRCs) consisting of rare PCBs congeners, that are assumed to not be present in the media in which the samplers were deployed, or present at concentrations so low as to be inconsequential and not affect calculations involving PRCs. The PRCs used for this project were: PCB-14, PCB-36, PCB-78, PCB-104, PCB-121, PCB-142, PCB-155, PCB-184, PCB-192, and PCB-204.

Each passive sampler was added to 500-mL amber glass jar containing a slurry composed of approximately 250 mL of wet sediment and 250 mL ultrapure water. Sodium azide (1 mL of a 25 gram per liter [g/L] aqueous solution) was added to each jar as a preservative to inhibit microbial transformation. Each sediment was evaluated via passive sampling via four replicates.

The jars were maintained at an average temperature of 20 degrees Celsius (°C) and rotated end-over-end at 27 rotations per minute (rpm) for 28 days. After the exposure period, samplers were removed from the jars, wrapped in aluminum foil, placed in an opaque resealable bag, then placed in an additional re-sealable plastic bag, and packaged in a cooler with ice packs for overnight shipment to a commercial chemical analytical laboratory (Eurofins TestAmerica). Three unexposed passive samplers (PRC control blanks) that remained in their original packaging under cold storage (approximately 4 °C) were also packaged for shipment in the same manner as the deployed samplers. These samplers were used to confirm the starting (time zero) concentration of PRCs in the sampler.

Processing of the samplers by TestAmerica included removal of the PE from the stainless-steel mesh envelope, removal of any visible sediment particles from the PE using a moist tissue, and solvent extraction of the PE (16 hours in a Soxhlet extractor using methylene chloride). After solvent cleanup and preconcentration, extracts were analyzed via Gas Chromatography/Mass Spectrometry Isotope Dilution methods consistent with USEPA Method 8270 (USEPA, 2018) to determine the concentrations of PCB congener PRCs and PAHs in PE.

Analyses of the four passive samplers exposed to the S (Urban Reference) sediment indicated that many of the results were undetectable. To improve the detection limit, two of the four solvent extracts were pooled and further concentrated to a smaller volume. Analysis of this single pooled extract was used to represent the concentration of PAHs and PRCs in the passive samplers exposed to the S (Urban Reference) sediment. In the future, when very low (e.g., ambient or trace) concentrations are expected, as in the case of the S (Urban Reference) sediment, a larger sampler should be used. For example, in the case of the PE design here, it can easily be increased from a 3- × 3-cm PE piece to a 5- × 5-cm PE piece. With the approximate 3-fold increase in PE mass, this can decrease the Method Detection Limit (MDL) by an approximate factor of 3. Based on a comparison of the analytical results of the pooled and concentrated samples and the original four samples, the reduction in MDL gained by using a larger sampler would have been sufficient to yield additional detections and would have been sufficient to indicate similar results as the concentrated samples.

The concentration of the PAHs and PRCs in PE were used in a multi-step data process to calculate C_{free} analytes. First, the concentrations of the PRCs in PE [PE_t] were used to calculate the elimination rate (k_e) values for the PRCs in each deployed sampler using the following equation (Lohmann, 2012):

$$PRC\ k_e = \ln\left(\frac{[PE_{t=0}]}{[PE_{t=final}]}\right) \div t_{final}$$

where:

$PE_{t=0}$ = the average concentration of the PRC present in the PE at the beginning of the deployment (obtained from an average measurement of the PRC control blanks)

$PE_{t=final}$ = the concentration of the PRC in the PE after the deployment (obtained from each deployed PE sampler)

t_{final} = the deployment time (in days)

k_e = the elimination rate (in $days^{-1}$)

The values are also expressed as a percentage of steady state (concentration at equilibrium).

The second step was to estimate k_e values for the PAHs (non-PRC PCB) in each of the deployed samplers. This was accomplished by developing a linear regression model using PRC k_e values (dependent variable) and PE-water partition coefficients (K_{PE}) for each PRC PCB (independent variable, Smedes et al., 2009). Note that regression models were specific to each sampler (i.e. not global to the whole deployment). Values were $\log_{10}$-transformed per Tomaszewski and Luthy (2008). By entering the analyte-specific K_{PE} into the linear regression model developed for each sampler, k_e values for each of the primary analytes for each sampler were calculated.

Third, concentrations of some non-PRC PCBs in PE were corrected for any trace levels of PAHs present in the unexposed PRC control blanks (due to trace levels present in the PRC spiking solutions). Using the sample specific k_e values, the expected amount of these trace primary analyte PCBs present in the sample at the end of deployment ($Trace\ PAH_{\ t\ =\ final}$) was calculated via the following equation:

$$[Trace\ PAH_{t\ =final}] = \frac{[Trace\ PAH_{t\ =\ 0}]}{e^{k_e \times\ t_{final}}}$$

where:

$Trace\ PAH_{t\ =\ final}$ = the concentration of trace PAHs remaining in the sample at the end of the deployment

$Trace\ PAH_{t\ =\ 0}$ = the average concentration of the trace PAHs in the PE at the beginning of the deployment (obtained from an average measurement of the trace PAHs in the PRC control blanks)

k_e = the elimination rate value predicted by the sampler-specific regression model (in $days^{-1}$)

t_{final} = the deployment time (in days)

Concentrations of $Trace\ PAH_{\ t\ =\ final}$ values were then subtracted from the measured concentrations of non-PRC PAHs in PE.

The fourth step describes the calculation of sampling rate correction factors (*CF*s) for each primary analyte in each sampler. The following equation is used, as adapted from Lohmann (2012):

$$CF\ = \frac{1}{1 - e^{-k_e \times\ t_{final}}}$$

where:

k_e = the elimination rate value predicted by the sampler-specific regression model (in $days^{-1}$)

t_{final} = the deployment time (in days).

The concentration of primary analyte in the PE of each sampler were then multiplied by the *CF* values to calculate the steady-state concentration of primary analytes.

In the final step, the steady-state concentrations are divided by K_{PE} values (Smedes et al., 2009) to obtain the concentrations of C_{free} for the primary analytes. C_{free} Method Detection Limits (MDLs) were calculated in the approach described above using the estimated MDL concentration in PE, as reported the analytical laboratory.

C_{free} results for each sample replicate, averages and SD values for the four test sediments are presented in Table S4.

Table S4. Freely-dissolved PAH concentration (C_{free}) as determined by passive samplers in the four test sediments. Where not detected, the MDL ("< value") are reported.

Analyte	PAH Type	Number of Rings	SI-4006-C-SP3-A	SI-4006-C-SP3-B	SI-4006-C-SP3-C	SI-4006-C-SP3-D	Average "C"	SD C	SI-4006-G2-SP3-A	SI-4006-G2-SP3-B	SI-4006-G2-SP3-C	SI-4006-G2-SP3-D	Average "G2"	SD G2	Average "S" (composite of replicates B & D)	SD S	SI-4006-V1-SP3-A	SI-4006-V1-SP3-B	SI-4006-V1-SP3-C	SI-4006-V1-SP3-D	Average "V1"	SD V1
			Result	Result	Result	Result	Mean	SD	Result	Result	Result	Result	Mean	SD	Mean	SD	Result	Result	Result	Result	Mean	SD
			(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)
Acenaphthene	Parent	3	< 60000	< 65000	< 60000	< 60000	0	0	280000	300000	280000	280000	285000	0	< 30000	NA	780000	5800000	4300000	3500000	3595000	2104939
Acenaphthylene	Parent	3	47000	< 54000	70000	< 47000	29250	35056	660000	660000	660000	600000	645000	0	< 26000	NA	1400000	1200000	1800000	1600000	1500000	258199
Anthracene	Parent	3	< 18000	< 20000	< 18000	< 18000	0	0	60000	53000	50000	56000	54750	0	< 9500	NA	2500000	4400000	7600000	5900000	5100000	2171021
Benzo[a]anthracene	Parent	4	< 1200	< 1200	< 920	1200	300	600	5900	6200	7300	5700	6275	0	< 500	NA	470000	450000	650000	490000	515000	91469
Benzo[a]pyrene	Parent	5	< 490	< 360	< 200	< 340	0	0	760	870	1300	880	952.5	0	< 98	NA	75000	72000	93000	83000	80750	9394
Benzo[b]fluoranthene	Parent	5	< 630	< 450	< 260	< 440	0	0	1000	1200	1900	1300	1350	0	< 130	NA	90000	97000	120000	110000	104250	13376
Benzo[e]pyrene	Parent	5	1100	700	580	780	790	222	< 800	870	< 1200	950	455	0	< 140	NA	41000	41000	49000	44000	43750	3775
Benzo[g,h,i]perylene	Parent	6	1500	370	290	550	677.5	559	240	290	910	400	460	0	< 9	NA	3100	2900	2900	2500	2850	252
Benzo[k]fluoranthene	Parent	5	< 410	< 290	< 170	< 290	0	0	490	620	870	< 500	495	0	< 83	NA	67000	60000	66000	57000	62500	4796
Chrysene	Parent	4	3000	3000	2400	3100	2875	320	20000	25000	24000	20000	22250	0	< 500	NA	260000	350000	390000	330000	332500	54391
Dibenz[a,h]anthracene	Parent	5	< 300	< 200	< 110	< 190	0	0	< 330	< 310	< 540	< 340	0	0	< 53	NA	7400	6300	8200	7800	7425	818
Fluoranthene	Parent	4	< 9400	< 11000	< 9400	< 9500	0	0	45000	47000	43000	40000	43750	0	5900	NA	8900000	8800000	12000000	9600000	9825000	1493039
Fluorene	Parent	3	< 37000	< 40000	< 37000	< 37000	0	0	420000	430000	450000	370000	417500	0	< 19000	NA	430000	1400000	1200000	1800000	1207500	575232
Indeno[1,2,3-cd]pyrene	Parent	6	< 350	< 190	< 97	< 200	0	0	< 330	340	< 620	370	177.5	0	< 44	NA	15000	13000	17000	14000	14750	1708
1-Methylnaphthalene	Alkylated	2	440000	< 260000	< 240000	< 240000	110000	220000	< 290000	< 240000	< 260000	< 240000	0	0	< 130000	NA	< 240000	580000	< 290000	580000	290000	334863
2-Methylnaphthalene	Alkylated	2	340000	< 340000	< 310000	< 310000	85000	170000	< 380000	< 310000	< 340000	< 310000	0	0	< 160000	NA	< 310000	< 310000	< 380000	< 340000	0	0
Naphthalene	Parent	2	5300000	< 1600000	< 1500000	< 1500000	1325000	2650000	< 1900000	< 1500000	< 1600000	< 1500000	0	0	1900000	NA	< 1500000	< 1500000	< 1900000	9200000	2300000	4600000
Perylene	Parent	5	< 590	< 420	< 240	< 410	0	0	3400	3800	5800	4000	4250	0	510	NA	16000	17000	19000	20000	18000	1826
Phenanthrene	Parent	3	< 100000	< 110000	< 100000	< 100000	0	0	440000	430000	380000	420000	417500	0	< 52000	NA	480000	880000	1300000	2400000	1265000	827426
Pyrene	Parent	4	9500	< 10000	< 9000	10000	4875	5633	36000	36000	29000	30000	32750	0	5000	NA	5500000	5200000	7700000	5800000	6050000	1126943
C1-Fluoranthenes/ pyrene	Alkylated	4	11000	11000	7700	12000	10425	1877	58000	67000	62000	49000	59000	0	< 2000	NA	1400000	1400000	1800000	1500000	1525000	189297
C1-Fluorenes	Alkylated	3	130000	110000	110000	120000	117500	9574	2300000	2500000	2600000	2300000	2425000	0	< 34000	NA	2400000	3300000	5500000	3500000	3675000	1307351
C2-Fluorenes	Alkylated	3	120000	110000	110000	140000	120000	14142	2200000	2400000	2200000	2100000	2225000	0	9900	NA	1200000	1300000	2000000	1300000	1450000	369685
C3-Fluorenes	Alkylated	3	73000	83000	76000	87000	79750	6397	940000	1100000	1000000	920000	990000	0	3600	NA	410000	390000	600000	450000	462500	95000
C2-Naphthalenes	Alkylated	2	< 300000	< 330000	< 300000	< 300000	0	0	16000000	20000000	18000000	17000000	17750000	0	< 160000	NA	1500000	3300000	3300000	2700000	2700000	848528
C3-Naphthalenes	Alkylated	2	480000	430000	420000	480000	452500	32016	13000000	15000000	15000000	13000000	14000000	0	< 54000	NA	2900000	3500000	7300000	3500000	4300000	2019901
C4-Naphthalenes	Alkylated	2	430000	410000	410000	460000	427500	23629	5500000	6100000	5600000	5000000	5550000	0	25000	NA	1700000	1700000	2900000	1800000	2025000	585235
C1-Phenanthrenes/ Anthracenes	Alkylated	3	35000	37000	33000	39000	36000	2582	650000	670000	570000	560000	612500	0	< 10000	NA	1200000	1400000	2000000	1500000	1525000	340343
C2-Phenanthrenes/ Anthracenes	Alkylated	3	71000	75000	62000	80000	72000	7616	910000	1000000	890000	820000	905000	0	6300	NA	1200000	1200000	1700000	1200000	1325000	250000

Table S4, continued.

Analyte	PAH Type	Number of Rings	SI-4006-C-SP3-A	SI-4006-C-SP3-B	SI-4006-C-SP3-C	SI-4006-C-SP3-D	Average "C"	SD C	SI-4006-G2-SP3-A	SI-4006-G2-SP3-B	SI-4006-G2-SP3-C	SI-4006-G2-SP3-D	Average "G2"	SD G2	Average "S" (composite of replicates B & D)	SD S	SI-4006-V1-SP3-A	SI-4006-V1-SP3-B	SI-4006-V1-SP3-C	SI-4006-V1-SP3-D	Average "V1"	SD V1
			Result	Result	Result	Result	Mean	SD	Result	Result	Result	Result	Mean	SD	Mean	SD	Result	Result	Result	Result	Mean	SD
			(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)	(pg/L)
C3-Phenanthrenes/ Anthracenes	Alkylated	3	59000	54000	51000	60000	56000	4243	470000	530000	540000	440000	495000	0	11000	NA	300000	280000	400000	340000	330000	52915
C4-Phenanthrenes/ Anthracenes	Alkylated	3	15000	11000	12000	12000	12500	1732	120000	140000	190000	130000	145000	0	3700	NA	43000	38000	51000	44000	44000	5354
C1-Chrysenes/ Benz[a]anthracenes	Alkylated	4	4200	2900	2600	3300	3250	695	31000	39000	49000	36000	38750	0	< 590	NA	200000	170000	230000	200000	200000	24495
C2-Chrysenes/ Benz[a]anthracenes	Alkylated	4	3300	1700	2100	< 1200	1775	1365	27000	32000	51000	32000	35500	0	< 340	NA	50000	42000	53000	45000	47500	4933
C3-Chrysenes/ Benz[a]anthracenes	Alkylated	4	1600	< 570	780	910	822.5	656	11000	13000	28000	15000	16750	0	< 110	NA	5300	4400	5600	4800	5025	532
C4-Chrysenes/ Benz[a]anthracenes	Alkylated	4	< 1100	< 320	240	< 400	60	120	4300	4900	16000	6900	8025	0	< 42	NA	660	430	660	490	560	118
Total C_{free} ΣPAH (pg/L)			7575200	1339670	1370690	1509840	**2948850**	3085121	44194090	51591090	48730080	44238500	**47188440**	3625293	**1970910**	**NA**	35543460	47394030	65155360	59622590	**51928860**	13205804
Total C_{free} ΣPAH (µg/L)			7.58	1.34	1.37	1.51	**2.95**	3.09	44.19	51.59	48.73	44.24	**47**	3.63	**1.97**	**NA**	35.54	47.39	65.16	59.62	**52**	13
Total C_{free}, 3-5 ring, ΣPAH_{3-5} (µg/L)			0.584	0.499	0.540	0.569	**0.55**	0.037	9.694	10.490	10.129	9.238	**10**	0.54	**0.046**	**NA**	29.425	38.298	51.635	41.826	**40**	9
% of 3-5 ring			8%	37%	39%	38%	**31%**	15%	22%	20%	21%	21%	**21%**	1%	**2%**	**NA**	83%	81%	79%	70%	**78%**	6%
Total C_{free} (µg/L), 2-ring PAHs			6.990	0.840	0.830	0.940	**2.400**	3.060	34.500	41.100	38.600	35.000	**37.300**	3.123	**1.925**	**NA**	6.100	9.080	13.500	17.780	**11.615**	5.112
Total C_{free} (µg/L), 3-ring PAHs			0.550	0.480	0.524	0.538	**0.523**	0.031	9.450	10.213	9.810	8.996	**9.617**	0.518	**0.035**	**NA**	12.343	21.588	28.451	23.534	**21.479**	6.741
Total C_{free} (µg/L), 4-ring PAHs			0.033	0.019	0.016	0.031	**0.024**	0.008	0.238	0.270	0.309	0.235	**0.263**	0.035	**0.011**	**NA**	16.786	16.417	22.829	17.970	**18.501**	2.961
Total C_{free} (µg/L), 5-ring PAHs			0.001	0.001	0.001	0.001	**0.001**	0.000	0.006	0.007	0.010	0.007	**0.008**	0.002	**0.001**	**NA**	0.296	0.293	0.355	0.322	**0.317**	0.029
Total C_{free} (µg/L), 6-ring PAHs			0.0015	0.0004	0.0003	0.0006	**0.001**	0.001	0.0002	0.0006	0.0009	0.0008	**0.001**	0.000	**0.0000**	**NA**	0.0181	0.0159	0.0199	0.0165	**0.018**	0.002
% of C_{free}, 2-ring PAHs			92%	63%	61%	62%	**69%**	15%	78%	80%	79%	79%	**79%**	1%	**98%**	**NA**	17%	19%	21%	30%	**22%**	6%
% of C_{free}, 3-ring PAHs			7%	36%	38%	36%	**29%**	15%	21%	20%	20%	20%	**20%**	1%	**2%**	**NA**	35%	46%	44%	39%	**41%**	5%
% of C_{free}, 4-ring PAHs			0.43%	1.39%	1.15%	2.02%	**1.25%**	0.66%	0.54%	0.52%	0.63%	0.53%	**0.56%**	0.05%	**0.55%**	**NA**	47.23%	34.64%	35.04%	30.14%	**37%**	7.32%
% of C_{free}, 5-ring PAHs			0.01%	0.05%	0.04%	0.05%	**0.04%**	0.02%	0.01%	0.01%	0.02%	0.02%	**0.02%**	0.00%	**0.03%**	**NA**	0.83%	0.62%	0.55%	0.54%	**0.63%**	0.14%
% of C_{free}, 6-ring PAHs			0.02%	0.03%	0.02%	0.04%	**0.03%**	0.01%	0.00%	0.00%	0.00%	0.00%	**0.00%**	0.00%	**0.00%**	**NA**	0.05%	0.03%	0.03%	0.03%	**0.04%**	0.01%

Notes

NA: Not Available, as only one passive sampling measurement per each PAH was made, precluding the calculation of SD values.
SD: Standard Deviation
Summed “Total” values were calculated by summing the detected PAHs.

3. Equilibrium Partitioning (EqP) Modeling to Predict C_{free}

For each PAH in each sediment, two predictions of C_{free} were made using two USEPA Equilibrium Partitioning (EqP) models.

The first approach, the 1-carbon model, assumes partitioning between TOC and sediment porewater, and is calculated using KOC values provided in USEPA (2012), the measured concentration of each PAH in sediment (Table S2), and the TOC content of in sediment (Table S2). It is estimated using the following equation (USEPA, 2012):

$$C_{free} = \frac{C_{sed}}{f_{OC}K_{OC}}$$

Where C_{sed} is concentration of the contaminant in sediment (µg/kg, dry weight (dw)), f_{OC} is the weight fraction of natural sedimentary organic carbon in sediment (kg OC/kg dw) represented by TOC in this investigation, and KOC is the TOC to water partition coefficient (L/kg TOC).

This second approach, the 2-carbon model, accounts for partitioning to the fraction of black carbon (f_{BC}) in sediment and the fraction of natural sedimentary organic carbon (f_{OC}). The two-carbon model can be used to calculate the C_{free} of PAHs using the following equation (USEPA, 2012):

$$C_{free} = \frac{C_{sed}}{f_{OC}K_{OC}+f_{BC}K_{BC}C_{free}^{n-1}}$$

Where C_{sed} is concentration of the contaminant in sediment (µg/kg), f_{OC} is the weight fraction of natural sedimentary organic carbon in sediment (kg OC/kg dw) represented by TOC in this investigation, fBC is the weight fraction of black carbon (BC) in sediment (g BC/g dw), K_{OC} is the TOC to water partition coefficient (L/kg TOC), K_{BC} is the BC to water partition coefficient (L/kg BC), and n is the Freundlich exponent, which accounts for non-linear sorption behavior (n = 0.6) (USEPA 2012).

According to USEPA (2012), the n-value of 0.6 has been used 1 for estimation the C_{free} of PAHs with Log Octanol-Water Partition Coefficients (Log K_{OW}s) between 4 and 5.5. Therefore this equation can be written as the following for PAHs:

$$f_{BC}K_{BC}{C_{free}}^{0.6} + f_{OC}K_{OC}C_{free} - C_{sed} = 0$$

This equation was further simplified by defining new parameters (a, b, c) and a variable x:

$$ax^{0.6} + bx - c = 0$$

Where:

x= C_{free}, a= $f_{BC} \times K_{BC}$, b= $f_{OC} \times K_{OC}$, c= C_{sed} of the PAH.

The Newton's method was implemented to solve Equation 6 for x as follows:

$$x_{m+1} = x_m + 0.5 \times \frac{ax^{0.6}+bx-c}{0.6\times x^{-0.4}+b}$$

Where m is the number of iterations and was set to be 10000. This equation was then solved with Matlab code to find the best estimation of x (C_{free}).

The 1-carbon and 2-carbon C_{free} model predictions for the PAHs are shown in Table S5. The 1-carbon C_{free} predictions for individual PAHs were an average (SD) of 4.8 (13) times higher than the 2-carbon C_{free} measurements. This is not surprising, as the 1-carbon model yields predictions that are often higher than that of the 2-carbon model, and it is recognized that the 1-carbon model often overestimates C_{free} (USEPA, 2012).

Table S5. Freely-dissolved PAH concentration (C_{free}) in the four test sediments, as predicted by 1-carbon and 2-carbon equilibrium partitioning models.

PAH	PAH Type	Number of Rings	C 1-carbon C_{free} (pg/L)	C 2-carbon C_{free} (pg/L)	G2 1-carbon C_{free} (pg/L)	G2 2-carbon C_{free} (pg/L)	S 1-carbon C_{free} (pg/L)	S 2-carbon C_{free} (pg/L)	V1 1-carbon C_{free} (pg/L)	V1 2-carbon C_{free} (pg/L)
Acenaphthene	Parent	3	51822	25564	731107	675360	55715	39312	48552987	46736000
Acenaphthylene	Parent	3	68972	31250	816632	758540	35291	23307	6219855	5628500
Anthracene	Parent	3	447522	289360	257224	229190	33764	22276	338319080	332010000
Benzo[a]anthracene	Parent	4	9545	1995	5985	3736	840	199	757088	609560
Benzo[a]pyrene	Parent	5	8019	1553	1849	897	423	73	491083	380470
Benzo[b]fluoranthene	Parent	5	8471	1666	4498	2656	966	242	1158191	963280
Benzo[g,h,i]perylene	Parent	6	24535	7805	598	209	224	29	79057	47774
Benzo[k]fluoranthene	Parent	5	2069	196	ND	ND	317	47	384615	290380
Chrysene	Parent	4	10472	2277	24250	18385	1145	309	902559	737010
Dibenz[a,h]anthracene	Parent	5	1073	73	99	16	10	0.2	15389	6249
Fluoranthene	Parent	4	16622	4313	81427	68223	24984	15871	10544793	9745200
Fluorene	Parent	3	78600	34402	1339243	1260300	58012	41121	99104017	95418000
Indeno[1,2,3-cd]pyrene	Parent	6	1017	68	82	12	21	1	23077	10628
Naphthalene	Parent	2	956127	652210	2997586	2875100	1144482	1029300	369155353	366360000
Phenanthrene	Parent	3	245107	141690	2155391	2051000	194511	157470	93352229	90156000
Pyrene	Parent	4	113913	56321	75890	63251	19337	11729	10799797	9986700
Perylene	Parent	5	727	42	4484	2669	2057	706	82188	49808
Benzo[e]pyrene	Parent	5	18869	5326	2342	1206	378	62	350773	262290
1-Methylnaphthalene	Alkylated	2	372128	228300	601565	552600	82254	60785	28535753	26732000
2-Methylnaphthalene	Alkylated	2	1023388	744550	1343077	1263800	134672	105060	84946724	81264000
C1-Fluoranthenes/ pyrene	Alkylated	4	72276	32033	72099	60096	2556	929	1832174	1570000
C1-Fluorenes	Alkylated	3	55423	22182	1100479	1032400	7056	3404	1916371	1639300
C2-Fluorenes	Alkylated	3	163179	87911	2472671	2361800	7387	3627	691626	549180
C3-Fluorenes	Alkylated	3	125401	63945	1111071	1043900	7019	3427	255415	182680
C2-Naphthalenes	Alkylated	2	610450	413560	21328976	20905000	76992	56762	17227250	16110000

Table S5, continued.

PAH	PAH Type	Number of Rings	C 1-carbon C_{free} (pg/L)	C 2-carbon C_{free} (pg/L)	G2 1-carbon C_{free} (pg/L)	G2 2-carbon C_{free} (pg/L)	S 1-carbon C_{free} (pg/L)	S 2-carbon C_{free} (pg/L)	V1 1-carbon C_{free} (pg/L)	V1 2-carbon C_{free} (pg/L)
C3-Naphthalenes	Alkylated	2	434112	281130	10547753	10277000	25179	15933	2905212	2543600
C4-Naphthalenes	Alkylated	2	150638	80314	1904313	1811100	5912	2762	243899	173510
C1-Phenanthrenes/ Anthracenes	Alkylated	3	174864	95551	930019	869030	33571	22350	2925607	2565600
C2-Phenanthrenes/ Anthracenes	Alkylated	3	239764	141030	1044019	979440	7537	3749	950860	777490
C3-Phenanthrenes/ Anthracenes	Alkylated	3	79310	36361	283784	255490	6341	3054	161538	109170
C4-Phenanthrenes/ Anthracenes	Alkylated	3	11722	2760	50113	40878	1357	402	19017	8176
C1-Chrysenes/ Benz[a]anthracenes	Alkylated	4	13765	3462	15413	11160	232	30	204717	143910
C2-Chrysenes/ Benz[a]anthracenes	Alkylated	4	5000	800	6057	3851	71	5	27886	13469
C3-Chrysenes/ Benz[a]anthracenes	Alkylated	4	1628	146	1325	610	12	0	3002	671
C4-Chrysenes/ Benz[a]anthracenes	Alkylated	4	328	12	243	63	2	0	327	23
Total C_{free} ΣPAH (pg/L)			**5596858**	**3490155**	**51311662**	**49478969**	**1970628**	**1624333**	**1123139511**	**1093780627**
Total C_{free} ΣPAH (µg/L)			**5.6**	**3.5**	**51**	**49**	**2.0**	**1.6**	**1123**	**1094**
Total C_{free}, 3-5 ring, ΣPAH_{3-5} (µg/L)			**2.0**	**1.1**	**12.6**	**11.8**	**0.5**	**0.4**	**620.0**	**600.5**
% of 3-5 ring			**36%**	**31%**	**25%**	**24%**	**25%**	**22%**	**55%**	**55%**

Notes

ND: Not Detected

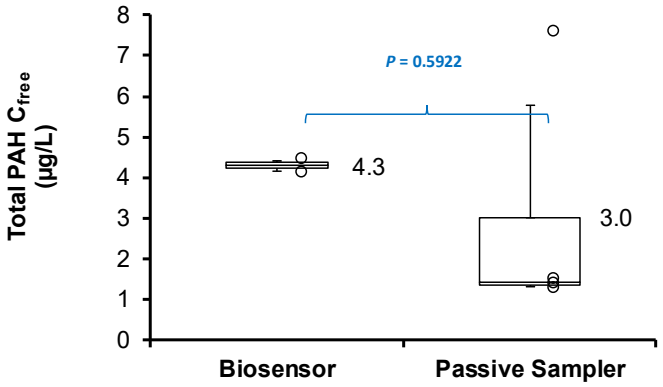
Summed "Total" values were calculated by summing the detected PAHs.

4. Statistical Summary of Predicted and Measured PAH C_{free}

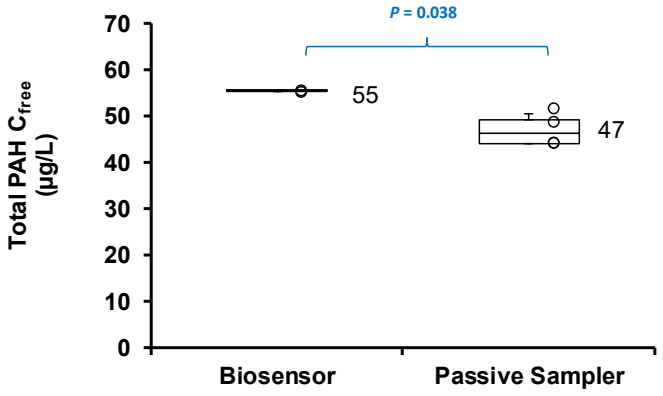
Summary statistics for C_{free} predictions and measurements are shown in Table S6.

Biosensor and passive sampler C_{free} ΣPAH results are compared statistically in Figure S2. Statistically significant differences were between the biosensor and passive sampler were found for the G2 and V1 sediments. If the highest C_{free} ΣPAH value for the C sediment (7.6 μg/L) is excluded as a potential outlier (Figure S2a), a statistical difference can be detected between the biosensor and passive sampler for this sediment (P = 0.0002).

(a)



(b)



(c)

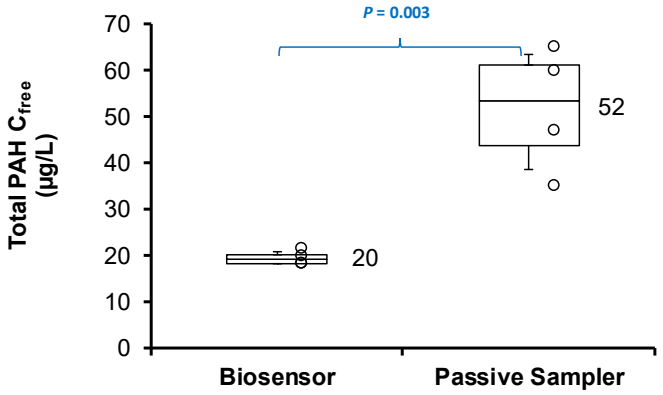


Figure S2. Sum of the total detected C_{free} PAHs (ΣPAH) and measured via passive samplers and the biosensor in three test sediments in which multiple measurements with both approaches were available: sediments C (a), G2 (b), and V1 (c). Value labels are the arithmetic mean, circle symbols are raw data, boxes are the interquartile range, and whiskers are the 10th and 90th percentiles.

Table S6. Sum of the total detected C_{free} PAHs (ΣPAH) and C_{free} 3- to 5-ring PAHs (ΣPAH_{3-5}) predicted by 1-carbon and 2-carbon EqP models and measured via passive samplers, and C_{free} ΣPAH measured via the biosensor in the four test sediments.

Sediment	1-carbon model		2-carbon model		Biosensor			Passive sampler					
	Total C_{free} (µg/L)	Total 3-5 Ring C_{free} (µg/L)	Total C_{free} (µg/L)	Total 3-5 Ring C_{free} (µg/L)	Total C_{free} (µg/L)			Total C_{free} (µg/L)			Total 3-5 Ring C_{free} (µg/L)		
	Single Value	Single Value	Single Value	Single Value	Mean	n	SD	Mean	n	SD	Mean	n	SD
C (Petroleum Low)	5.6	2.0	3.5	1.1	4.3	2	0.22	2.9	4	3.1	0.55	4	0.037
G2 (Petroleum High)	51	13	49	12	55	2	0.21	47	4	3.6	9.9	4	0.54
S (Urban Reference)	2.0	0.50	1.6	0.35	3.1	2	0.18	2.0	1	NA	0.046	1	NA
V1 (Creosote)	1123	620	1094	601	20	4	1.5	52	4	13	40	4	9.2

Notes
NA: Not Available.
n: Number of replicates
SD: Standard Deviation
Summed "Total" values were calculated by summing the detected PAHs.

5. PAH Patterns

PAH histograms for the sediments indicated the typical histogram patterns for the two petroleum (C, G2) and creosote (V1) sediments, as shown in Figure S3. For example, the two petroleum (C, G2) sediments indicated higher levels of alkylated naphthalenes and alkylated chrysenes relative to their respective parent PAHs (Figure S3a and Figure S3b), indicating a typical petrogenic PAH signature (Neff et al., 2005). In contrast, the creosote (V1) sediment indicated the converse: higher concentrations of chrysene and naphthalenes relative to their respective alkylated PAH groups (Figure S2c), indicating a typical pyrogenic PAH signature. These patterns were not as evident in histograms created using C_{free} data (Figure S4). Resolving and understanding PAH sources is likely to be more difficult than using bulk "total" analysis since patterns are affected by large differences in PAH-specific partitioning (driven largely by hydrophobicity) and differences in the types of organic carbon present in sediments, which can greatly influence partitioning (Ghosh et al., 2003).

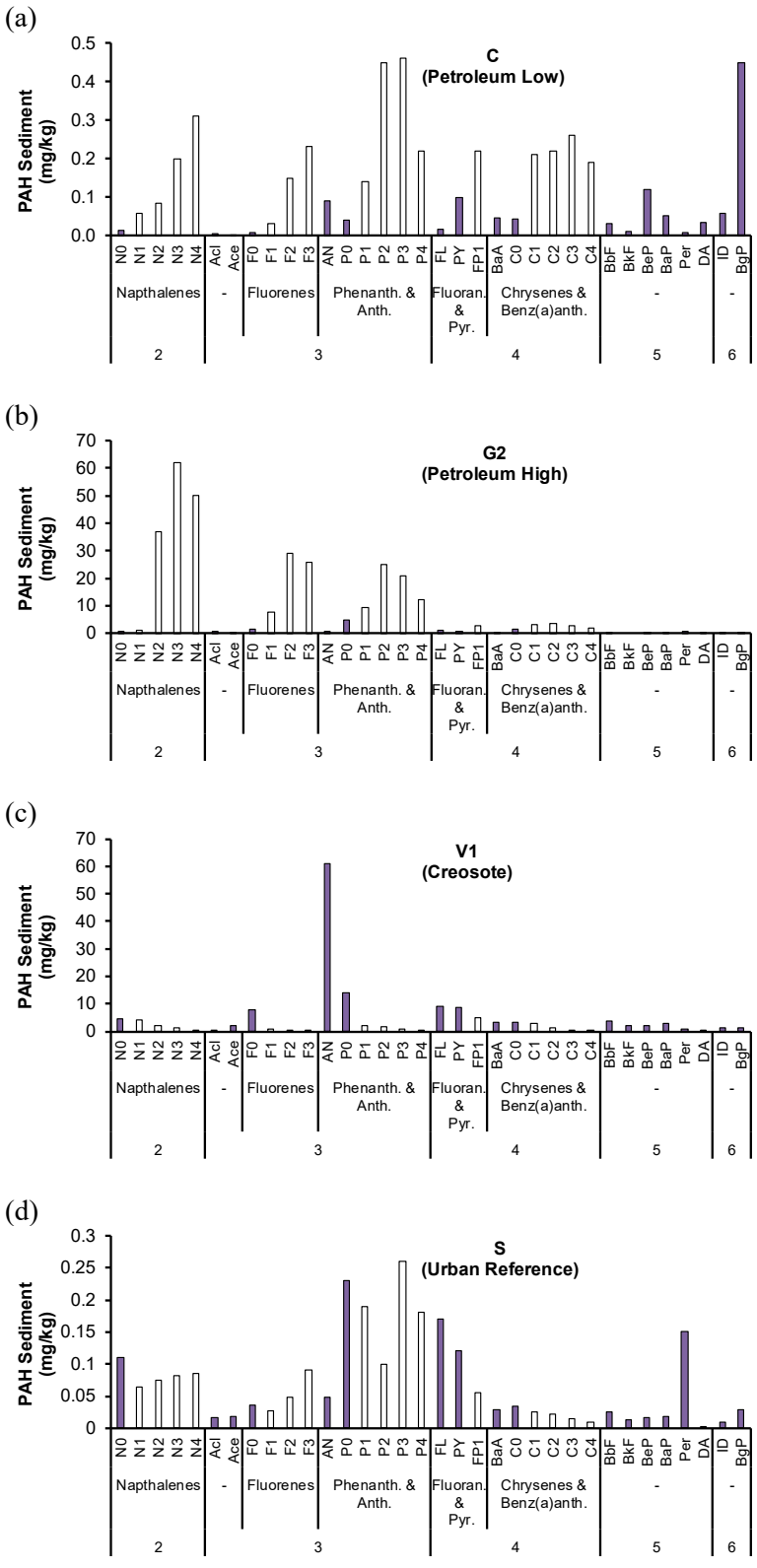


Figure S3. PAH histograms based on total concentrations of PAHs in sediment (values from Table S2). Parent PAHs are shown with solid bars; alkylated PAHs are shown with hollow bars.

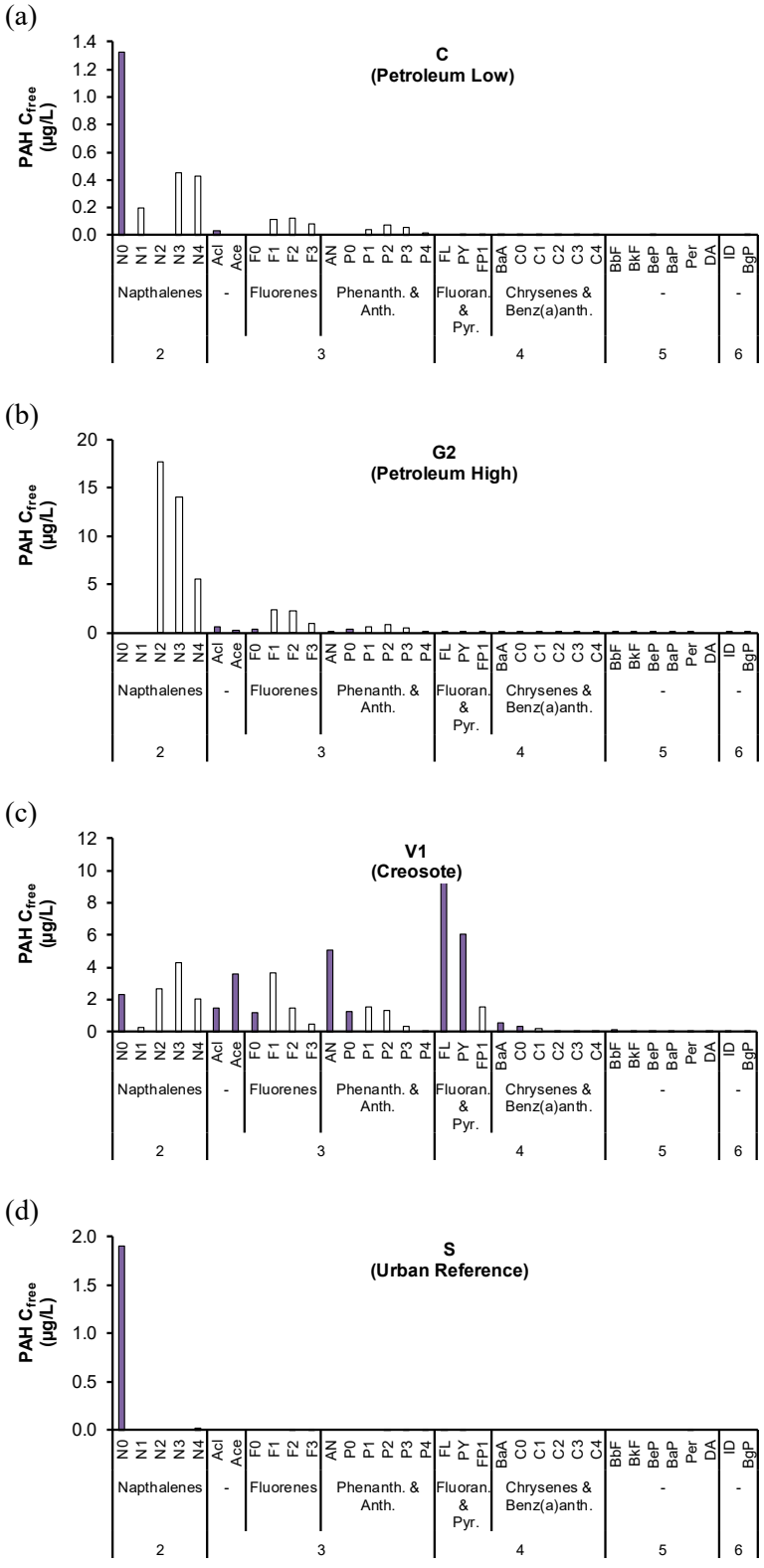


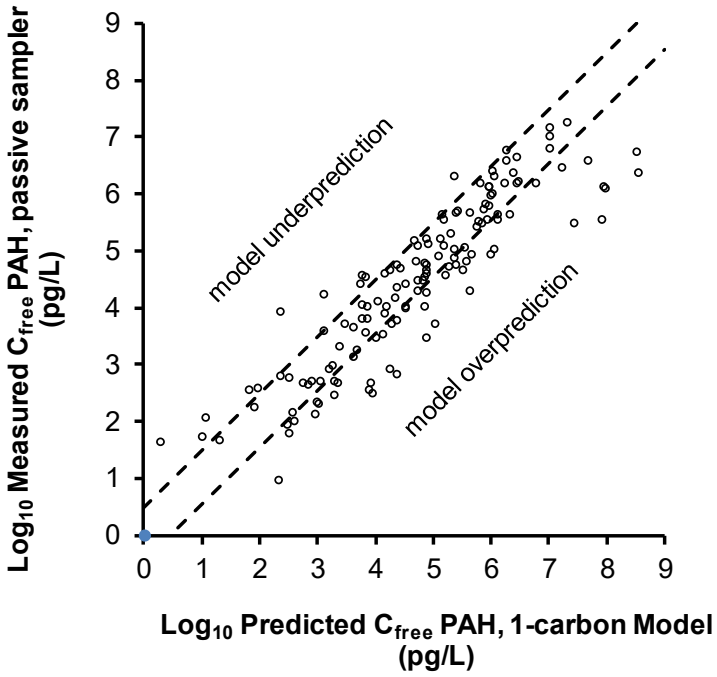
Figure S4. PAH histograms based on C_{free} PAHs measured with passive samplers (mean values from Table S4). Parent PAHs are shown with solid bars; alkylated PAHs are shown with hollow bars.

6. EqP Model Predictions versus C_{free} Measurements via Passive Sampling

PAH C_{free} predictions derived from the 1-carbon and 2-carbon EqP models (Table S5) were compared to mean C_{free} measurements via passive sampling for individual PAHs (Figure S5). Among the predicted and measured C_{free} values for individual PAHs in all four test sediments (Figure S5), 1-carbon and 2-carbon models overestimated measured Cfree values by a mean (SD) of 9 (29) and 7 (27), respectively. 56% and 57% of 1-carbon and 2-carbon model predictions for the individual PAH C_{free} values, respectively, were within a factor of 3 of measured values.

All mean C_{free} measurements were obtained from Table S4 except for those in which all C_{free} measurements did not indicate detectable PAHs (i.e., mean values of 0 in Table S4, comprising 30% of the 140 mean C_{free} values). In these cases, the mean Log_{10} of the MDLs in the samples was used as the passive sampler C_{free} value in Figure S5. Because actual C_{free} values are below these values, it is likely that the EqP models overestimate the actual C_{free} measurements to a higher degree than suggested in Figure S5 and as discussed in the main text.

(a)



(b)

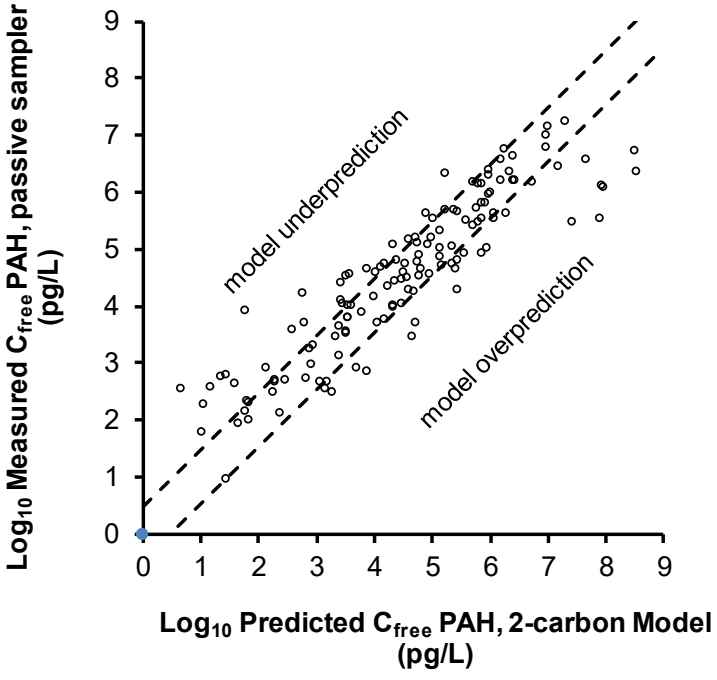


Figure S5. Mean Log_{10}-transformed C_{free} PAHs measured with passive samplers compared to 1-carbon (a) and 2-carbon (b) EqP model predictions. Points between the diagonal dashed lines indicate agreement within a factor of 3 or less between measured and predicted values.

7. Calculation of Toxic Units from Measured and Predicted C_{free}

Toxic Units (TU) were calculated for each PAH by dividing the C_{free} values measured by passive sampling (Table S4) by PAH Final Chronic Values (FCVs; USEPA (2003)), as shown in Table S7. In cases in a particular PAH was not detected, a value of 0 was reported for the TU. The sum of the TU (ΣTU) were calculated by summing the individual PAH TUs for a sample. The same approach was used to calculate TU and ΣTU based on C_{free} predictions of the 1-carbon and 2-carbon equilibrium partitioning models (Table S5), as shown in Table S8.

Table S7. Toxic Units calculated using freely-dissolved PAH concentration (C_{free}) measured by passive samplers (Table S4) and USEPA Final Chronic Values (USEPA, 2003).

Analyte	PAH Type	Number of Rings	USEPA Final Chronic Value (FCV) (pg/L) USEPA (2003)	SI-4006-C-SP3-A	SI-4006-C-SP3-B	SI-4006-C-SP3-C	SI-4006-C-SP3-D	Average "C"	SD C	SI-4006-G2-SP3-A	SI-4006-G2-SP3-B	SI-4006-G2-SP3-C	SI-4006-G2-SP3-D	Average "G2"	SD G2	Average "S" (composite of replicates B & D)	SD S	SI-4006-V1-SP3-A	SI-4006-V1-SP3-B	SI-4006-V1-SP3-C	SI-4006-V1-SP3-D	Average "V1"	SD V1
Acenaphthene	Parent	3	5.6E+07	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.0E-03	5.4E-03	5.0E-03	5.0E-03	5.1E-03	1.8E-04	0.0E+00	NA	1.4E-02	1.0E-01	7.7E-02	6.3E-02	6.4E-02	3.8E-02
Acenaphthylene	Parent	3	3.1E+08	1.5E-04	0.0E+00	2.3E-04	0.0E+00	9.5E-05	1.1E-04	2.2E-03	2.2E-03	2.2E-03	2.0E-03	2.1E-03	9.8E-05	0.0E+00	NA	4.6E-03	3.9E-03	5.9E-03	5.2E-03	4.9E-03	8.4E-04
Anthracene	Parent	3	2.1E+07	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.9E-03	2.6E-03	2.4E-03	2.7E-03	2.6E-03	2.1E-04	0.0E+00	NA	1.2E-01	2.1E-01	3.7E-01	2.8E-01	2.5E-01	1.0E-01
Benzo[a]anthracene	Parent	4	2.2E+06	0.0E+00	0.0E+00	0.0E+00	5.4E-04	1.3E-04	2.7E-04	2.6E-03	2.8E-03	3.3E-03	2.6E-03	2.8E-03	3.2E-04	0.0E+00	NA	2.1E-01	2.0E-01	2.9E-01	2.2E-01	2.3E-01	4.1E-02
Benzo[a]pyrene	Parent	5	9.6E+05	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	7.9E-04	9.1E-04	1.4E-03	9.2E-04	9.9E-04	2.5E-04	0.0E+00	NA	7.8E-02	7.5E-02	9.7E-02	8.7E-02	8.4E-02	9.8E-03
Benzo[b]fluoranthene	Parent	5	6.8E+05	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.5E-03	1.8E-03	2.8E-03	1.9E-03	2.0E-03	5.7E-04	0.0E+00	NA	1.3E-01	1.4E-01	1.8E-01	1.6E-01	1.5E-01	2.0E-02
Benzo[e]pyrene	Parent	5	9.0E+05	1.2E-03	7.8E-04	6.4E-04	8.7E-04	8.8E-04	2.5E-04	0.0E+00	9.7E-04	0.0E+00	1.1E-03	5.1E-04	5.8E-04	0.0E+00	NA	4.6E-02	4.6E-02	5.4E-02	4.9E-02	4.9E-02	4.2E-03
Benzo[g,h,i]perylene	Parent	6	4.4E+05	3.4E-03	8.4E-04	6.6E-04	1.3E-03	1.5E-03	1.3E-03	5.5E-04	6.6E-04	2.1E-03	9.1E-04	1.0E-03	7.0E-04	0.0E+00	NA	7.1E-03	6.6E-03	6.6E-03	5.7E-03	6.5E-03	5.7E-04
Benzo[k]fluoranthene	Parent	5	6.4E+05	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	7.6E-04	9.7E-04	1.4E-03	0.0E+00	7.7E-04	5.7E-04	0.0E+00	NA	1.0E-01	9.4E-02	1.0E-01	8.9E-02	9.7E-02	7.5E-03
Chrysene	Parent	4	2.0E+06	1.5E-03	1.5E-03	1.2E-03	1.5E-03	1.4E-03	1.6E-04	9.8E-03	1.2E-02	1.2E-02	9.8E-03	1.1E-02	1.3E-03	0.0E+00	NA	1.3E-01	1.7E-01	1.9E-01	1.6E-01	1.6E-01	2.7E-02
Dibenz[a,h]anthracene	Parent	5	2.8E+05	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	NA	2.6E-02	2.2E-02	2.9E-02	2.8E-02	2.6E-02	2.9E-03
Fluoranthene	Parent	4	7.1E+06	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.3E-03	6.6E-03	6.0E-03	5.6E-03	6.2E-03	4.2E-04	8.3E-04	NA	1.3E+00	1.2E+00	1.7E+00	1.4E+00	1.4E+00	2.1E-01
Fluorene	Parent	3	3.9E+07	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.1E-02	1.1E-02	1.1E-02	9.4E-03	1.1E-02	8.7E-04	0.0E+00	NA	1.1E-02	3.6E-02	3.1E-02	4.6E-02	3.1E-02	1.5E-02
Indeno[1,2,3-cd]pyrene	Parent	6	2.8E+05	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.2E-03	0.0E+00	1.3E-03	6.5E-04	7.5E-04	0.0E+00	NA	5.5E-02	4.7E-02	6.2E-02	5.1E-02	5.4E-02	6.2E-03
1-Methylnaphthalene	Alkylated	2	7.5E+07	5.8E-03	0.0E+00	0.0E+00	0.0E+00	1.5E-03	2.9E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	NA	0.0E+00	7.7E-03	0.0E+00	7.7E-03	3.8E-03	4.4E-03
2-Methylnaphthalene	Alkylated	2	7.2E+07	4.7E-03	0.0E+00	0.0E+00	0.0E+00	1.2E-03	2.4E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	NA	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Naphthalene	Parent	2	1.9E+08	2.7E-02	0.0E+00	0.0E+00	0.0E+00	6.8E-03	1.4E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	9.8E-03	NA	0.0E+00	0.0E+00	0.0E+00	4.8E-02	1.2E-02	2.4E-02
Perylene	Parent	5	9.0E+05	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	3.8E-03	4.2E-03	6.4E-03	4.4E-03	4.7E-03	1.2E-03	5.7E-04	NA	1.8E-02	1.9E-02	2.1E-02	2.2E-02	2.0E-02	2.0E-03
Phenanthrene	Parent	3	1.9E+07	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.3E-02	2.2E-02	2.0E-02	2.2E-02	2.2E-02	1.4E-03	0.0E+00	NA	2.5E-02	4.6E-02	6.8E-02	1.3E-01	6.6E-02	4.3E-02
Pyrene	Parent	4	1.0E+07	9.4E-04	0.0E+00	0.0E+00	9.9E-04	4.8E-04	5.6E-04	3.6E-03	3.6E-03	2.9E-03	3.0E-03	3.2E-03	3.7E-04	4.9E-04	NA	5.4E-01	5.1E-01	7.6E-01	5.7E-01	6.0E-01	1.1E-01
C1-Fluoranthenes/ pyrene	Alkylated	4	4.9E+06	2.3E-03	2.3E-03	1.6E-03	2.5E-03	2.1E-03	3.8E-04	1.2E-02	1.4E-02	1.3E-02	1.0E-02	1.2E-02	1.6E-03	0.0E+00	NA	2.9E-01	2.9E-01	3.7E-01	3.1E-01	3.1E-01	3.9E-02
C1-Fluorenes	Alkylated	3	1.4E+07	9.3E-03	7.9E-03	7.9E-03	8.6E-03	8.4E-03	6.8E-04	1.6E-01	1.8E-01	1.9E-01	1.6E-01	1.7E-01	1.1E-02	0.0E+00	NA	1.7E-01	2.4E-01	3.9E-01	2.5E-01	2.6E-01	9.3E-02
C2-Fluorenes	Alkylated	3	5.3E+06	2.3E-02	2.1E-02	2.1E-02	2.6E-02	2.3E-02	2.7E-03	4.1E-01	4.5E-01	4.1E-01	4.0E-01	4.2E-01	2.4E-02	1.9E-03	NA	2.3E-01	2.5E-01	3.8E-01	2.5E-01	2.7E-01	7.0E-02
C3-Fluorenes	Alkylated	3	1.9E+06	3.8E-02	4.3E-02	4.0E-02	4.5E-02	4.2E-02	3.3E-03	4.9E-01	5.7E-01	5.2E-01	4.8E-01	5.2E-01	4.2E-02	1.9E-03	NA	2.1E-01	2.0E-01	3.1E-01	2.3E-01	2.4E-01	5.0E-02
C2-Naphthalenes	Alkylated	2	3.0E+07	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.3E-01	6.6E-01	6.0E-01	5.6E-01	5.9E-01	5.6E-02	0.0E+00	NA	5.0E-02	1.1E-01	1.1E-01	8.9E-02	8.9E-02	2.8E-02
C3-Naphthalenes	Alkylated	2	1.1E+07	4.3E-02	3.9E-02	3.8E-02	4.3E-02	4.1E-02	2.9E-03	1.2E+00	1.4E+00	1.4E+00	1.2E+00	1.3E+00	1.0E-01	0.0E+00	NA	2.6E-01	3.2E-01	6.6E-01	3.2E-01	3.9E-01	1.8E-01
C4-Naphthalenes	Alkylated	2	4.0E+06	1.1E-01	1.0E-01	1.0E-01	1.1E-01	1.1E-01	5.8E-03	1.4E+00	1.5E+00	1.4E+00	1.2E+00	1.4E+00	1.1E-01	6.2E-03	NA	4.2E-01	4.2E-01	7.2E-01	4.4E-01	5.0E-01	1.4E-01
C1-Phenanthrenes/ Anthracenes	Alkylated	3	7.4E+06	4.7E-03	5.0E-03	4.4E-03	5.2E-03	4.8E-03	3.5E-04	8.7E-02	9.0E-02	7.7E-02	7.5E-02	8.2E-02	7.5E-03	0.0E+00	NA	1.6E-01	1.9E-01	2.7E-01	2.0E-01	2.1E-01	4.6E-02
C2-Phenanthrenes/ Anthracenes	Alkylated	3	3.2E+06	2.2E-02	2.3E-02	1.9E-02	2.5E-02	2.3E-02	2.4E-03	2.8E-01	3.1E-01	2.8E-01	2.6E-01	2.8E-01	2.3E-02	2.0E-03	NA	3.8E-01	3.8E-01	5.3E-01	3.8E-01	4.1E-01	7.8E-02
C3-Phenanthrenes/ Anthracenes	Alkylated	3	1.3E+06	4.7E-02	4.3E-02	4.1E-02	4.8E-02	4.5E-02	3.4E-03	3.7E-01	4.2E-01	4.3E-01	3.5E-01	3.9E-01	3.8E-02	8.8E-03	NA	2.4E-01	2.2E-01	3.2E-01	2.7E-01	2.6E-01	4.2E-02

Table S7, continued.

Analyte	PAH Type	Number of Rings	USEPA Final Chronic Value (FCV) (pg/L) USEPA (2003)	SI-4006-C-SP3-A	SI-4006-C-SP3-B	SI-4006-C-SP3-C	SI-4006-C-SP3-D	Average "C"	SD C	SI-4006-G2-SP3-A	SI-4006-G2-SP3-B	SI-4006-G2-SP3-C	SI-4006-G2-SP3-D	Average "G2"	SD G2	Average "S" (composite of replicates B & D)	SD S	SI-4006-V1-SP3-A	SI-4006-V1-SP3-B	SI-4006-V1-SP3-C	SI-4006-V1-SP3-D	Average "V1"	SD V1
C4-Phenanthrenes/ Anthracenes	Alkylated	3	5.6E+05	2.7E-02	2.0E-02	2.1E-02	2.1E-02	2.2E-02	3.1E-03	2.1E-01	2.5E-01	3.4E-01	2.3E-01	2.6E-01	5.6E-02	6.6E-03	NA	7.7E-02	6.8E-02	9.1E-02	7.9E-02	7.9E-02	9.6E-03
C1-Chrysenes/ Benz[a]anthracenes	Alkylated	4	8.6E+05	4.9E-03	3.4E-03	3.0E-03	3.9E-03	3.8E-03	8.1E-04	3.6E-02	4.6E-02	5.7E-02	4.2E-02	4.5E-02	8.9E-03	0.0E+00	NA	2.3E-01	2.0E-01	2.7E-01	2.3E-01	2.3E-01	2.9E-02
C2-Chrysenes/ Benz[a]anthracenes	Alkylated	4	4.8E+05	6.8E-03	3.5E-03	4.4E-03	0.0E+00	3.7E-03	2.8E-03	5.6E-02	6.6E-02	1.1E-01	6.6E-02	7.4E-02	2.2E-02	0.0E+00	NA	1.0E-01	8.7E-02	1.1E-01	9.3E-02	9.8E-02	1.0E-02
C3-Chrysenes/ Benz[a]anthracenes	Alkylated	4	1.7E+05	9.6E-03	0.0E+00	4.7E-03	5.4E-03	4.9E-03	3.9E-03	6.6E-02	7.8E-02	1.7E-01	9.0E-02	1.0E-01	4.6E-02	0.0E+00	NA	3.2E-02	2.6E-02	3.3E-02	2.9E-02	3.0E-02	3.2E-03
C4-Chrysenes/ Benz[a]anthracenes	Alkylated	4	7.1E+04	0.0E+00	0.0E+00	3.4E-03	0.0E+00	8.5E-04	1.7E-03	6.1E-02	6.9E-02	2.3E-01	9.8E-02	1.1E-01	7.7E-02	0.0E+00	NA	9.3E-03	6.1E-03	9.3E-03	6.9E-03	7.9E-03	1.7E-03
Total Toxic Units				**0.39**	**0.32**	**0.31**	**0.35**	**0.34**	**0.04**	**5.4**	**6.2**	**6.2**	**5.3**	**5.77**	**0.49**	**0.04**	**NA**	**5.6**	**6.0**	**8.6**	**6.6**	**6.69**	**1.33**
Total Toxic Units, 2-ring PAHs				0.187	0.140	0.139	0.157	**0.16**	0.02	3.059	3.520	3.330	2.969	**3.22**	0.25	**0.016**		0.731	0.852	1.483	0.905	**0.99**	0.34
Total Toxic Units, 3-ring PAHs				0.171	0.163	0.154	0.180	**0.17**	0.01	2.074	2.324	2.288	1.996	**2.17**	0.16	**0.021**		1.639	1.940	2.841	2.180	**2.15**	0.51
Total Toxic Units, 4-ring PAHs				0.026	0.011	0.018	0.015	**0.02**	0.01	0.253	0.298	0.593	0.327	**0.37**	0.15	**0.001**		2.799	2.730	3.722	2.975	**3.06**	0.46
Total Toxic Units, 5-ring PAHs				0.001	0.001	0.001	0.001	**0.00**	0.00	0.007	0.009	0.012	0.008	**0.01**	0.00	**0.001**		0.405	0.399	0.482	0.437	**0.43**	0.04
Total Toxic Units, 6-ring PAHs				0.003	0.001	0.001	0.001	**0.00**	0.00	0.001	0.002	0.002	0.002	**0.00**	0.00	**0.000**		0.062	0.054	0.068	0.057	**0.06**	0.01
Total Toxic Units, 3-5 ring				0.198	0.174	0.173	0.196	**0.19**	0.01	2.334	2.630	2.893	2.331	**2.55**	0.27	**0.023**		4.843	5.069	7.045	5.592	**5.64**	0.99
% of Toxic Units, 2-ring PAHs				48%	44%	44%	44%	**45%**	1.9%	57%	57%	53%	56%	**56%**	1.7%	**41%**		13%	14%	17%	14%	**15%**	1.9%
% of Toxic Units, 3-ring PAHs				44%	52%	49%	51%	**49%**	3.5%	38%	38%	37%	38%	**38%**	0.7%	**54%**		29%	32%	33%	33%	**32%**	2.0%
% of Toxic Units, 4-ring PAHs				6.7%	3.4%	5.8%	4.2%	**5%**	1.5%	4.7%	4.8%	9.5%	6.2%	**6%**	2.2%	**3.4%**		49.7%	45.7%	43.3%	45.4%	**46%**	2.7%
% of Toxic Units, 5-ring PAHs				0.3%	0.2%	0.2%	0.2%	**0.3%**	0.0%	0.1%	0.1%	0.2%	0.2%	**0.2%**	0.0%	**1.5%**		7.2%	6.7%	5.6%	6.7%	**7%**	0.7%
% of Toxic Units, 6-ring PAHs				0.9%	0.3%	0.2%	0.4%	**0.4%**	0.3%	0.0%	0.0%	0.0%	0.0%	**0.0%**	0.0%	**0.0%**		1.1%	0.9%	0.8%	0.9%	**0.9%**	0.1%
% of Toxic Units, 3-5 ring PAHs				51%	55%	55%	55%	**54%**	2.2%	43%	43%	46%	44%	**44%**	1.6%	**59%**		86%	85%	82%	85%	**85%**	2%

Notes
NA: Not Available.
SD: Standard Deviation
Summed “Total” values were calculated by summing the detected PAHs.

Table S8. Toxic Units calculated using freely-dissolved PAH concentration (C_{free}) predicted by 1-carbon and 2-carbon equilibrium partitioning models (Table S5) and USEPA Final Chronic Values (USEPA, 2003).

Analyte	PAH Type	Number of Rings	USEPA Final Chronic Value (FCV) (pg/L) USEPA (2003)	C 1-carbon	C 2-carbon	G2 1-carbon	G2 2-carbon	S 1-carbon	S 2-carbon	V1 1-carbon	V1 2-carbon
Acenaphthene	Parent	3	5.6E+07	9.3E-04	4.6E-04	1.3E-02	1.2E-02	1.0E-03	7.0E-04	8.7E-01	8.4E-01
Acenaphthylene	Parent	3	3.1E+08	2.2E-04	1.0E-04	2.7E-03	2.5E-03	1.1E-04	7.6E-05	2.0E-02	1.8E-02
Anthracene	Parent	3	2.1E+07	2.2E-02	1.4E-02	1.2E-02	1.1E-02	1.6E-03	1.1E-03	1.6E+01	1.6E+01
Benzo[a]anthracene	Parent	4	2.2E+06	4.3E-03	9.0E-04	2.7E-03	1.7E-03	3.8E-04	8.9E-05	3.4E-01	2.7E-01
Benzo[a]pyrene	Parent	5	9.6E+05	8.4E-03	1.6E-03	1.9E-03	9.4E-04	4.4E-04	7.6E-05	5.1E-01	4.0E-01
Benzo[b]fluoranthene	Parent	5	6.8E+05	1.3E-02	2.5E-03	6.6E-03	3.9E-03	1.4E-03	3.6E-04	1.7E+00	1.4E+00
Benzo[g,h,i]perylene	Parent	6	4.4E+05	5.6E-02	1.8E-02	1.4E-03	4.8E-04	5.1E-04	6.5E-05	1.8E-01	1.1E-01
Benzo[k]fluoranthene	Parent	5	6.4E+05	3.2E-03	3.1E-04	0.0E+00	0.0E+00	4.9E-04	7.4E-05	6.0E-01	4.5E-01
Chrysene	Parent	4	2.0E+06	5.1E-03	1.1E-03	1.2E-02	9.0E-03	5.6E-04	1.5E-04	4.4E-01	3.6E-01
Dibenz[a,h]anthracene	Parent	5	2.8E+05	3.8E-03	2.6E-04	3.5E-04	5.7E-05	3.7E-05	5.6E-07	5.4E-02	2.2E-02
Fluoranthene	Parent	4	7.1E+06	2.3E-03	6.1E-04	1.1E-02	9.6E-03	3.5E-03	2.2E-03	1.5E+00	1.4E+00
Fluorene	Parent	3	3.9E+07	2.0E-03	8.8E-04	3.4E-02	3.2E-02	1.5E-03	1.0E-03	2.5E+00	2.4E+00
Indeno[1,2,3-cd]pyrene	Parent	6	2.8E+05	3.7E-03	2.5E-04	3.0E-04	4.5E-05	7.6E-05	2.7E-06	8.4E-02	3.9E-02
Naphthalene	Parent	2	1.9E+08	4.9E-03	3.4E-03	1.5E-02	1.5E-02	5.9E-03	5.3E-03	1.9E+00	1.9E+00
Phenanthrene	Parent	3	1.9E+07	1.3E-02	7.4E-03	1.1E-01	1.1E-01	1.0E-02	8.2E-03	4.9E+00	4.7E+00
Pyrene	Parent	4	1.0E+07	1.1E-02	5.6E-03	7.5E-03	6.3E-03	1.9E-03	1.2E-03	1.1E+00	9.9E-01
Perylene	Parent	5	9.0E+05	8.1E-04	4.7E-05	5.0E-03	3.0E-03	2.3E-03	7.8E-04	9.1E-02	5.5E-02
Benzo[e]pyrene	Parent	5	9.0E+05	2.1E-02	5.9E-03	2.6E-03	1.3E-03	4.2E-04	6.9E-05	3.9E-01	2.9E-01
1-Methylnaphthalene	Alkylated	2	7.5E+07	4.9E-03	3.0E-03	8.0E-03	7.3E-03	1.1E-03	8.1E-04	3.8E-01	3.5E-01
2-Methylnaphthalene	Alkylated	2	7.2E+07	1.4E-02	1.0E-02	1.9E-02	1.8E-02	1.9E-03	1.5E-03	1.2E+00	1.1E+00
C1-Fluoranthenes/pyrene	Alkylated	4	4.9E+06	1.5E-02	6.6E-03	1.5E-02	1.2E-02	5.2E-04	1.9E-04	3.7E-01	3.2E-01
C1-Fluorenes	Alkylated	3	1.4E+07	4.0E-03	1.6E-03	7.9E-02	7.4E-02	5.0E-04	2.4E-04	1.4E-01	1.2E-01
C2-Fluorenes	Alkylated	3	5.3E+06	3.1E-02	1.7E-02	4.7E-01	4.5E-01	1.4E-03	6.8E-04	1.3E-01	1.0E-01
C3-Fluorenes	Alkylated	3	1.9E+06	6.5E-02	3.3E-02	5.8E-01	5.4E-01	3.7E-03	1.8E-03	1.3E-01	9.5E-02
C2-Naphthalenes	Alkylated	2	3.0E+07	2.0E-02	1.4E-02	7.1E-01	6.9E-01	2.5E-03	1.9E-03	5.7E-01	5.3E-01

Table S8, continued.

Analyte	PAH Type	Number of Rings	USEPA Final Chronic Value (FCV) (pg/L) USEPA (2003)	C 1-carbon	C 2-carbon	G2 1-carbon	G2 2-carbon	S 1-carbon	S 2-carbon	V1 1-carbon	V1 2-carbon
C3-Naphthalenes	Alkylated	2	1.1E+07	3.9E-02	2.5E-02	9.5E-01	9.3E-01	2.3E-03	1.4E-03	2.6E-01	2.3E-01
C4-Naphthalenes	Alkylated	2	4.0E+06	3.7E-02	2.0E-02	4.7E-01	4.5E-01	1.5E-03	6.8E-04	6.0E-02	4.3E-02
C1-Phenanthrenes/ Anthracenes	Alkylated	3	7.4E+06	2.4E-02	1.3E-02	1.3E-01	1.2E-01	4.5E-03	3.0E-03	3.9E-01	3.5E-01
C2-Phenanthrenes/ Anthracenes	Alkylated	3	3.2E+06	7.5E-02	4.4E-02	3.3E-01	3.1E-01	2.4E-03	1.2E-03	3.0E-01	2.4E-01
C3-Phenanthrenes/ Anthracenes	Alkylated	3	1.3E+06	6.3E-02	2.9E-02	2.3E-01	2.0E-01	5.0E-03	2.4E-03	1.3E-01	8.7E-02
C4-Phenanthrenes/ Anthracenes	Alkylated	3	5.6E+05	2.1E-02	4.9E-03	9.0E-02	7.3E-02	2.4E-03	7.2E-04	3.4E-02	1.5E-02
C1-Chrysenes/ Benz[a]anthracenes	Alkylated	4	8.6E+05	1.6E-02	4.0E-03	1.8E-02	1.3E-02	2.7E-04	3.5E-05	2.4E-01	1.7E-01
C2-Chrysenes/ Benz[a]anthracenes	Alkylated	4	4.8E+05	1.0E-02	1.7E-03	1.3E-02	8.0E-03	1.5E-04	9.9E-06	5.8E-02	2.8E-02
C3-Chrysenes/ Benz[a]anthracenes	Alkylated	4	1.7E+05	9.7E-03	8.7E-04	7.9E-03	3.6E-03	7.4E-05	1.8E-06	1.8E-02	4.0E-03
C4-Chrysenes/ Benz[a]anthracenes	Alkylated	4	7.1E+04	4.6E-03	1.6E-04	3.4E-03	9.0E-04	3.0E-05	2.3E-07	4.6E-03	3.3E-04
Total Toxic Units				**0.63**	**0.29**	**4.3**	**4.1**	**0.063**	**0.038**	**38**	**35**

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